Large Eddy Simulation of Flow-Field and Micro-Particle Deposition in an Idealized Mouth-Throat and Constricted Tube

X.G. Cui, E. Gutheil*
Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

Abstract
The study concerns the simulation of the flow field and particle transport in the upper human respiratory system. The numerical simulations are conducted using large eddy simulation and a Lagrangian particle tracking method. The average velocity at the centerline and at different cross-sections in the constricted tube is compared with the data from literature [1]. Moreover, the particle deposition efficiency in the idealized mouth-throat is analyzed and compared with data from the literature [1]. The main properties of the flow field in the idealized geometry are captured in the present numerical results. Future work will include the simulation of a human mouth-throat obtained from CT scans the numerical grid of which will be shown and discussed in the paper.

Introduction

Particle deposition in human respiratory system has great influence on human health such as toxical particle inhalation from the environment and targeted drugs for treating lung disease. Many numerical simulations have been done to study the property of flow field and particle deposition. The flow field and micro-particle transport in an idealized geometry was simulated by Zhang et al. [1]. The results exhibit the main features of transitional laminar-turbulent flows including particle suspension in the human oral airways. It also shows that the turbulence may enchance the particle deposition in the treachea near the larynx in particular for the particle deposition of smaller particles. Jin et al. [2] found that turbulent dispersion plays an import role on the particle deposition for the particle with small Stokes number. They found that particles with the diameter of 1 μm not only deposites on the opposite wall but also on the side wall. The deposition patterns in a CT based realistic air-way model were analyzed by Jayarajua et al. [3]. The realistic airway flow simulations show that the laminar to turbulent transition, especially at low flow rates, is sensitive to the complexity of the airway model. Flow transition is seen soon after the glottis region for a low flow rate of 15 L/min, which are not reported in the simplified geometry simulations [3]. The paper focuses on simulating the flow field and micro-particle deposition in the simplified geometry with large eddy simulation using the Smargorinsky subgrid model [5]. To evaluate the methodology, the comparison was done with the data from the literature [1]. Further work will be developed on the basis. A complex numerical grid will be shown which is generated from CT scans, and both the surface grid as well as the computational grid is discussed.

Methodology

Based on the diameter variations along the oral airway from mouth to trachea and the coordinate of points in the centerline [4], the circular simplified geometry has been generated using Ansys ICEM-CFD 11.0. Neglecting the influence of particles on the fluid, the three-dimensional incompressible Navier-Stokes equations are solved to depict the flow field. Large eddy simulation (LES) is used to treat the turbulence, and the sub-grid scale (SGS) model introduced by Smargorinsky, 1963 is adopted [5]. Assuming large particle-to-air density ratio, negligible particle rotation, no inter-particle collision, and drag force as the dominant point force, the Lagrangian equations are used to describe particle motion [2]. To solve these equations, the software platform OpenFOAM 1.5 (http://www.opencfd.co.uk/Openfoam/) is used. A new solver, which can solve the flow field with LES and particle motion using a Lagrangian formulation is reconstructed based on the solver of oodles and icolagrancianFoam (www.openfoamwiki.net).

Results and Discussion

First, the flow field in a simple constricted tube transiting from laminar to turbulent is modeled and compared with data from the literature [1, 6]. The number of grid nodes for the present simulation is 1,043,955. The velocity on the inlet surface is given as 0.473 m/s with 2 %, corresponding to Re_{in}=2,000. The relative pressure on the outlet is zero. The axial velocity on the centerline is shown in Figure 1. Here, the velocity is normalized by the inlet velocity, and the distance is normalized by diameter D and R, respectively. From the comparison, it

* Corresponding author: gutheil@iwr.uni-heidelberg.de

can be seen that our result fit well with both the numerical and experimental results along the centerline [1]. The velocity profile in different cross section is compared with the numerical and experimental results. They will be discussed in the full paper.

Moreover, the flow field at normal breathing with 30 L/min is simulated. At present, the number of grid nodes is 219,849. The boundary condition is the same as the case of flow field in the constricted tube. The average velocity in the mid-plane is shown in the Fig. 2, it can be seen that the simulation captures the main properties of flow field in the oral airway, such as the skewed velocity profile in the oral cavity, and pharynx; flow separation in the lower portion of mouth, in the pharynx region after the soft palate, and downstream of glottis; asymmetric laryngeal jet generating after the glottis. In fact, there are numerical results for the inspiration rate at 15 L/min and 60 L/min. They will be discussed in the paper.

Particle motion is simulated on a coarser grid with 103,443 nodes. The particle deposition efficiency is 3,000 based on the impaction parameter ($\rho d_p^2 Q$) at an inspiration flow rate of 30 L/min for a particle diameter of 10 µm. The deposition efficiency is 54.2 % very close to the value of 53.3 % in the literature [1]. More results on the particle deposition comparison will be presented in the full paper.

From the comparison for the velocity on the centerline of the constricted tube, it is concluded that the present methodology adequately predicts the flow field transition from laminar to turbulent. The average velocity contour in the mid-plane shows that the methodology is suitable to capture the complex structure in the idealized geometry. Moreover, the present method adequately predicts the micro-particle deposition.

Acknowledgement

The authors gratefully acknowledge financial support of the German Science Foundation (DFG) through International Graduate College 710. They thank Dr. Rhode and Prof. Baumann from Heidelberg Medical School for providing the CT scans and Mr. Jungblut for generating the surface grid from the CT data.

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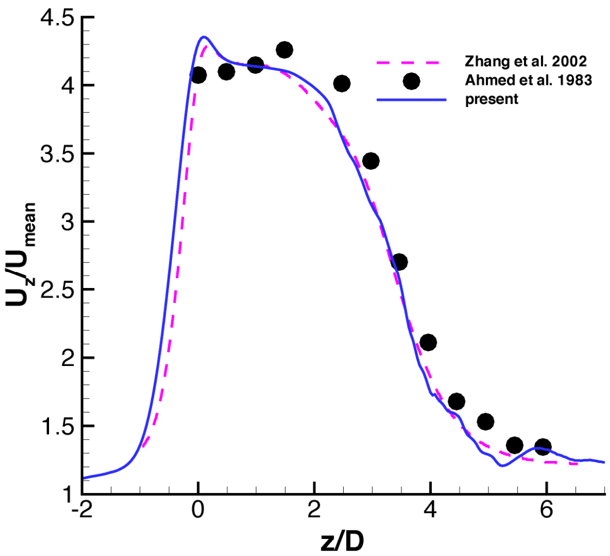

Figure 1. Comparison of the normalized centerline velocity for a constricted tube with numerical [1] and experimental data [6].

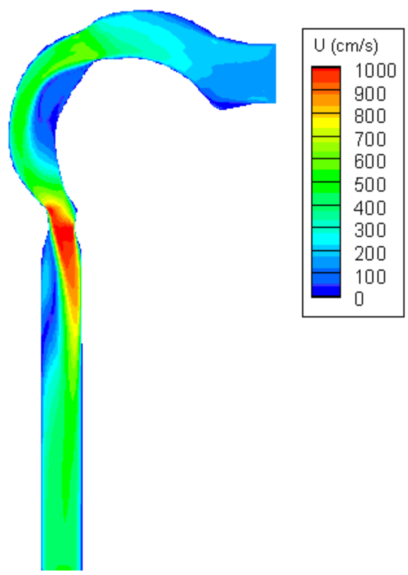

Figure 2. Velocity contours at the mid-plane.